# Elastic Moduli and Vibrational Modes in Jammed Sphere Packings

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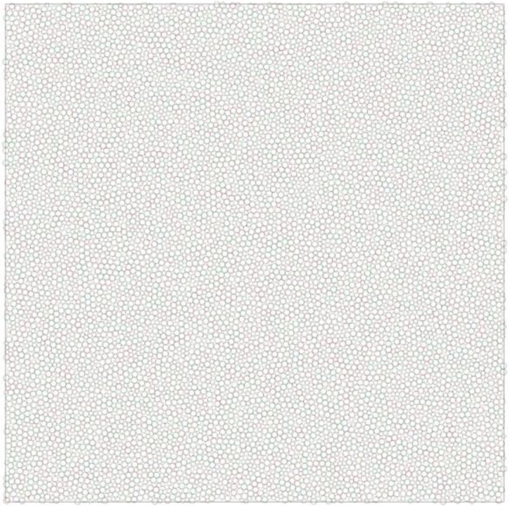
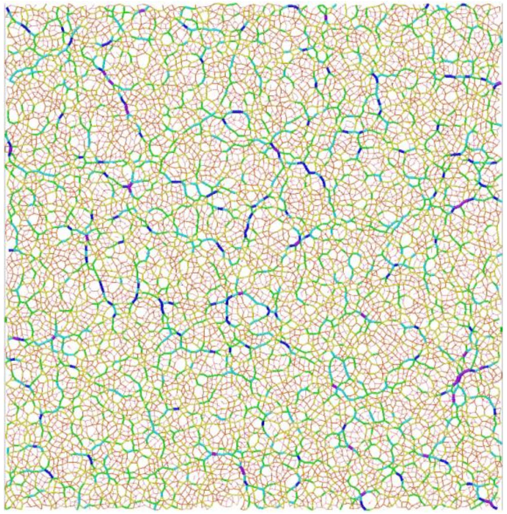
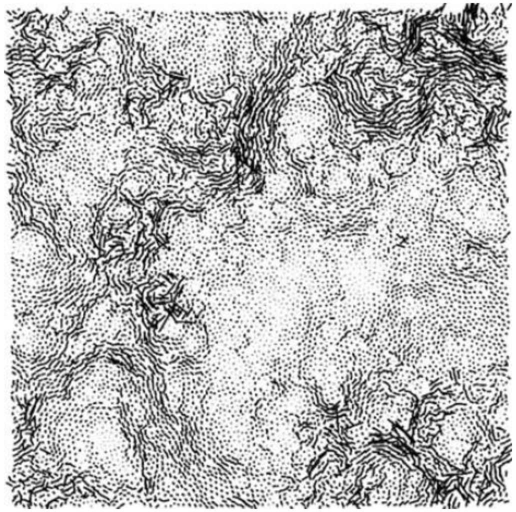
Particles



Forces



Normal modes

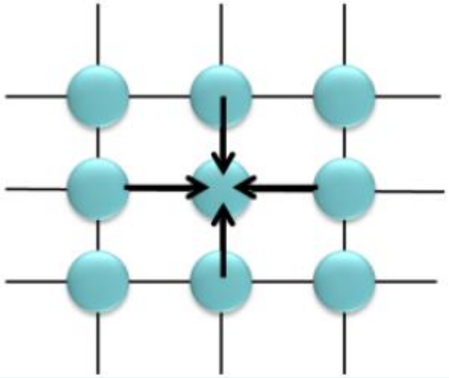


Avalanches, plasticity, and nonlinear response in nonequilibrium solids March 7th – 9th, 2016

14:15-14:40 Monday 7th, March, 2016

# Elastic response of amorphous solid

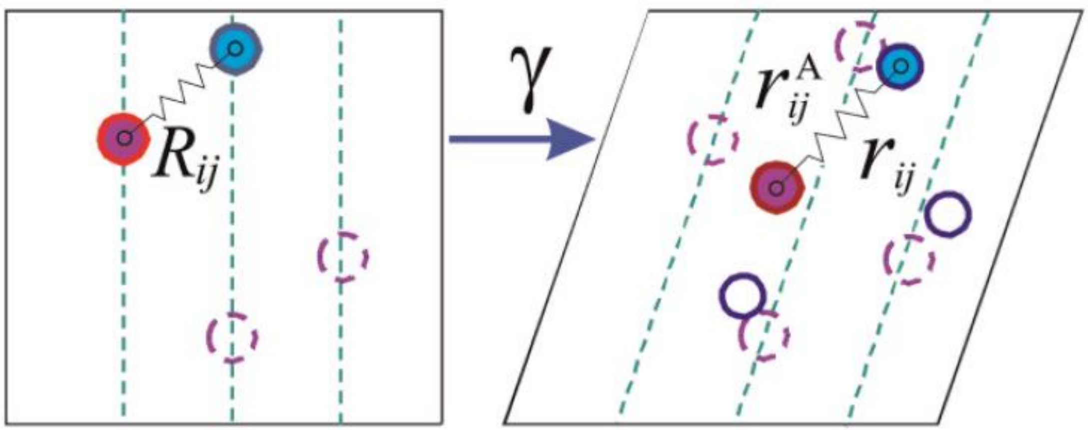
- Apply affine deformation on system
- In (one component) **perfect crystal**, particles follow the affine strain field
- In **amorphous solid**, force unbalance causes an additional relaxation



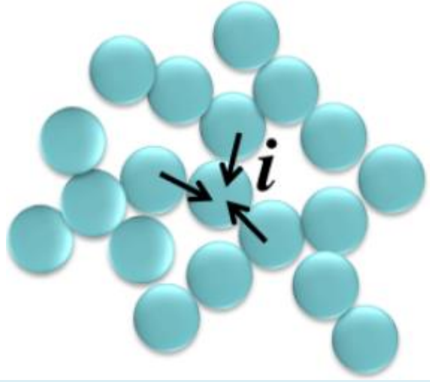
**Perfect lattice structure**

⇒ Particles follow the affine strain field with no additional relaxation

Affine deformation




Zaccone and Terentjev, PRL (2013)

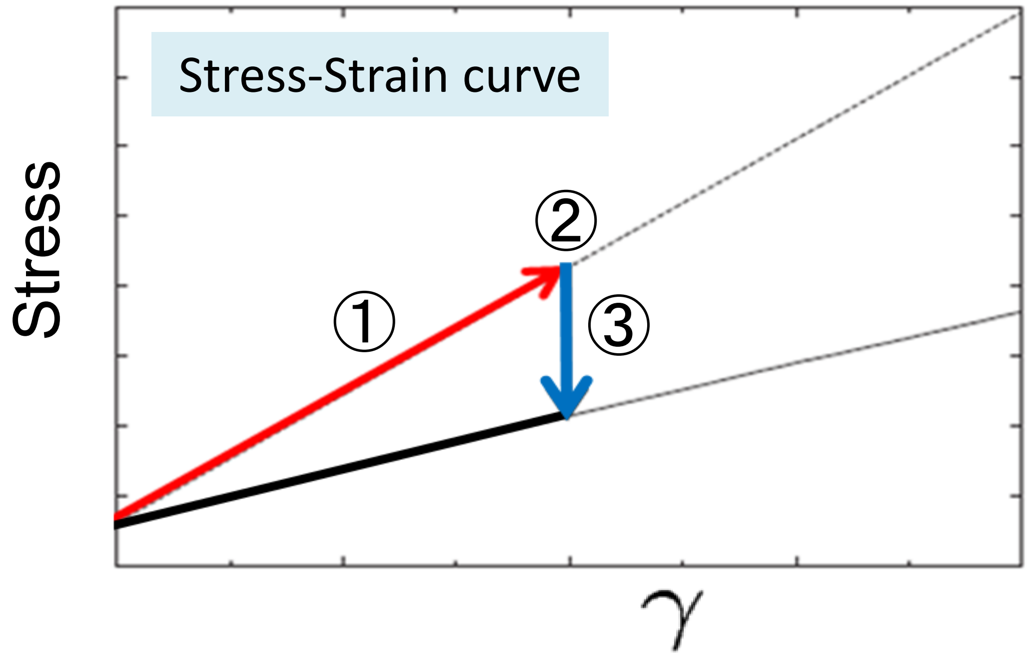



**Amorphous structure**

⇒ Affine deformation causes force unbalance, driving an additional non-affine relaxation

# Elastic response of amorphous solid

① Deform the system affinely ⇒ rescale all coordinates $X \to X(1+\gamma)$
② **Force unbalances** are induced between particles
③ Undergo an additional **non-affine relaxation** $X(1+\gamma) \to X'$




Elastic modulus = **Affine** + **Non-affine**

$$G = G_A - G_N$$

⇒ Non-affine relaxation decreases modulus (non-affine contribution)

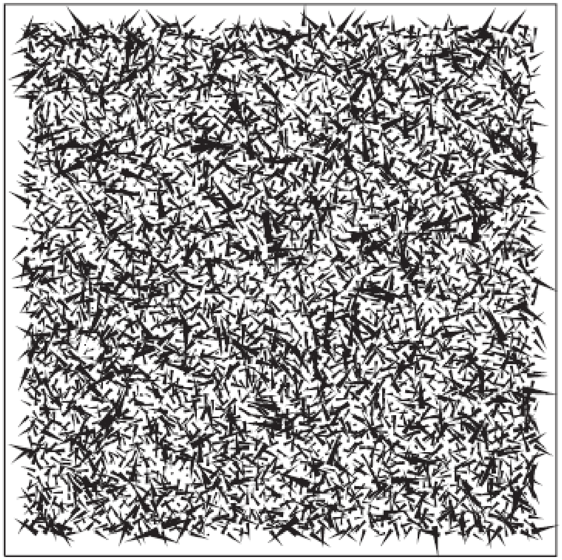
# Elastic response of amorphous solid

① Deform the system affinely ⇒ rescale all coordinates $X \to X(1+\gamma)$

② **Force unbalances** are induced between particles

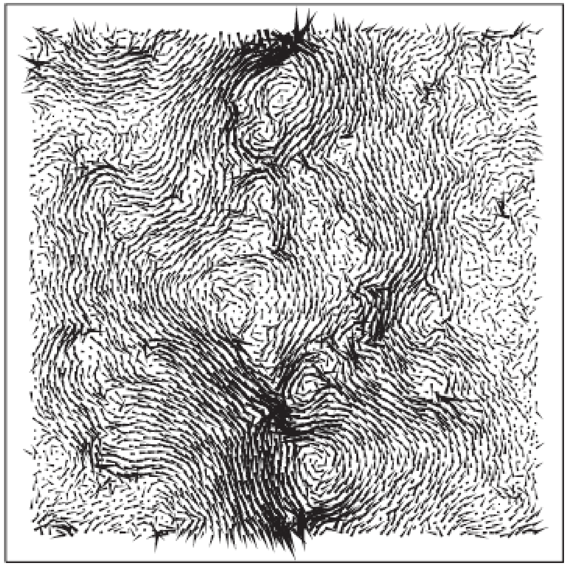
③ Undergo an additional **non-affine relaxation** $X(1+\gamma) \to X'$

**Forces** acting on particles induced by affine deformation



Random distribution with short-range correlation

**Particle displacements** driven by forces, during non-affine relaxation



Vortex-like structure with long-range correlation

C.E. Maloney, PRL (2006)

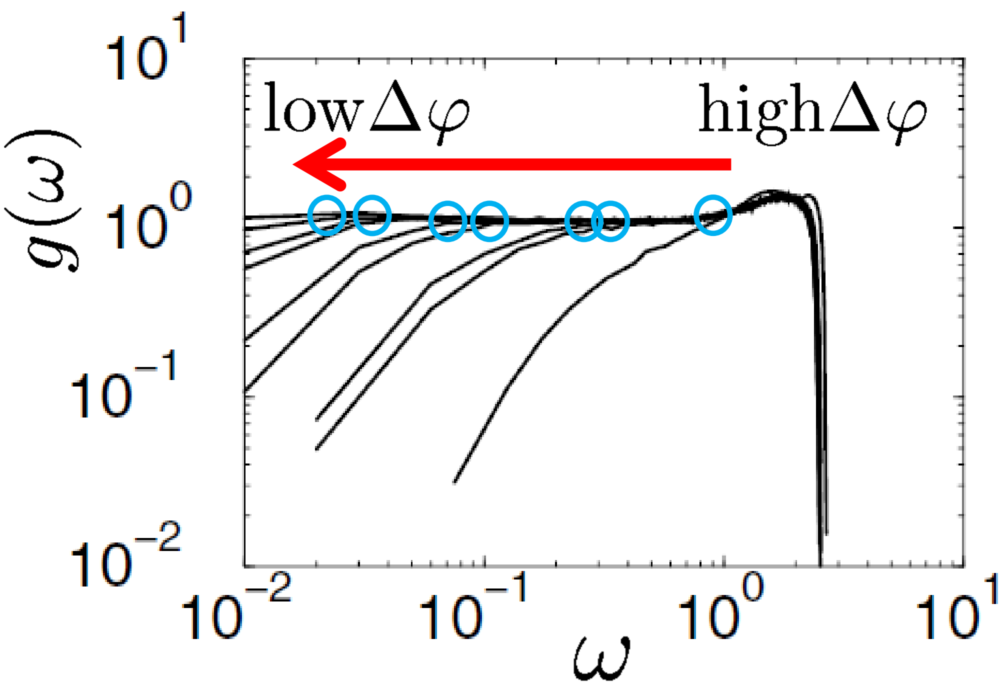
During non-affine relaxation, **vibrational normal modes** are excited !

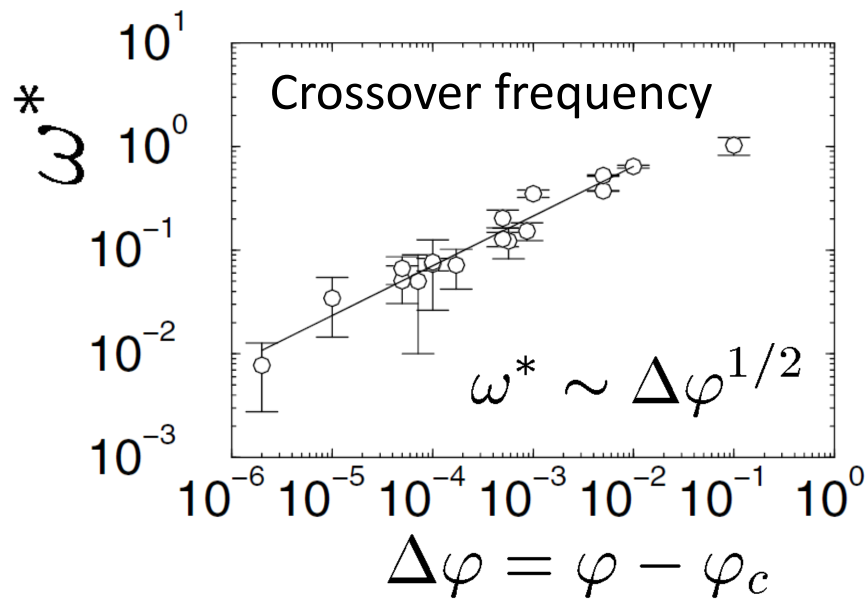
# Vibrational normal modes – Density of states

- Harmonic potential
- Frictionless particles

$$\phi(r_{ij}) = \begin{cases} \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{\sigma}\right)^2 & (r_{ij} < \sigma) \\ 0 & (r_{ij} \geq \sigma) \end{cases}$$

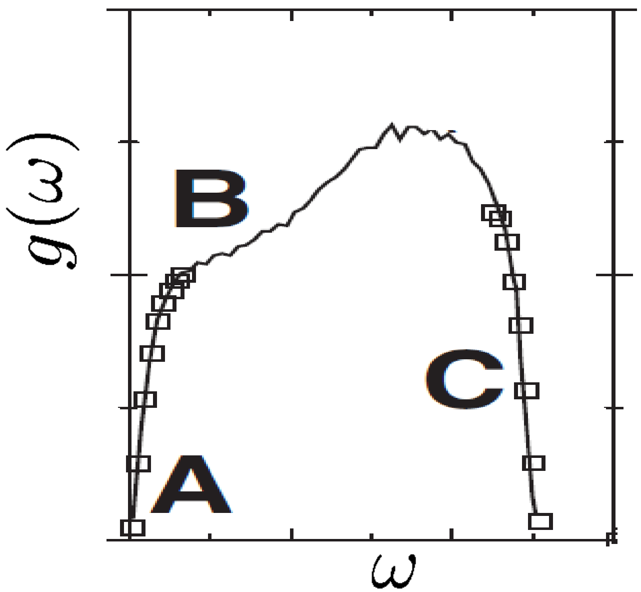
- Crossover at $\omega^*$ from **Debye-like regime** to **plateau regime**
- On approach to jamming transition point $\varphi_c$, **plateau regime** extends towards zero frequency: $\omega^* \sim \Delta\varphi^{1/2} \to 0$



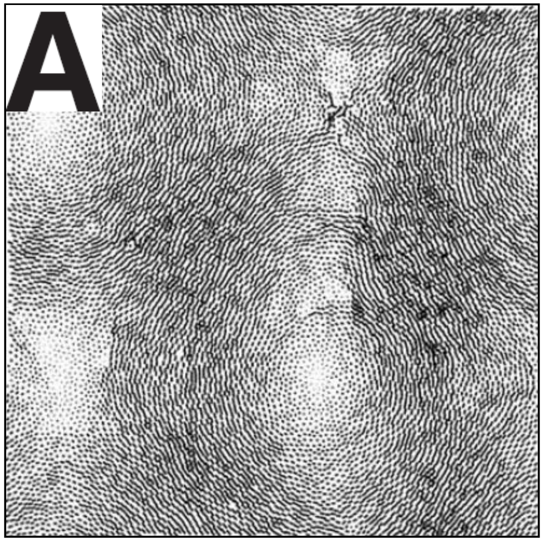

L.E. Silbert et al., PRL (2005)

# Vibrational normal modes – Polarization vector $e^k$

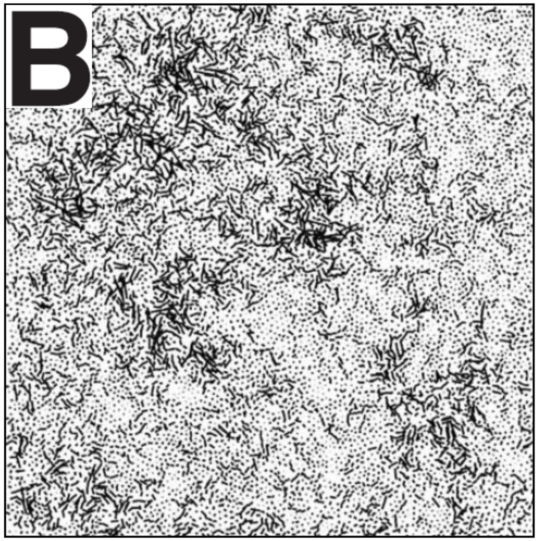



- **A, Debye-like regime :**
  Some plane-wave-like character
- **B, Plateau regime :**
  Filamentary nature of extented mode
- **C, High frequency regime :**
  Truely, highly localized mode

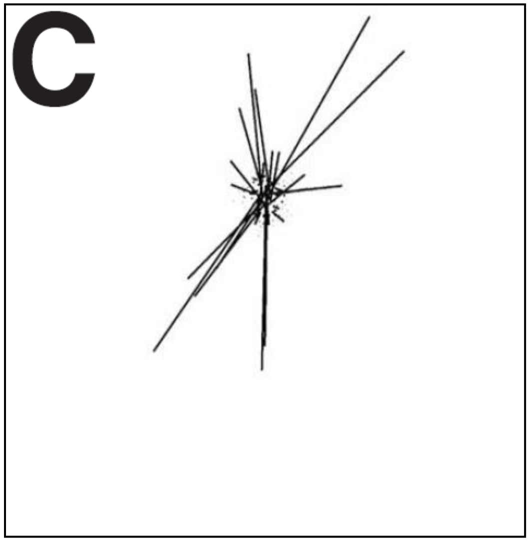
L.E. Silbert et al., PRE (2009)




Plane-wave-like modes




Filamentary extended modes



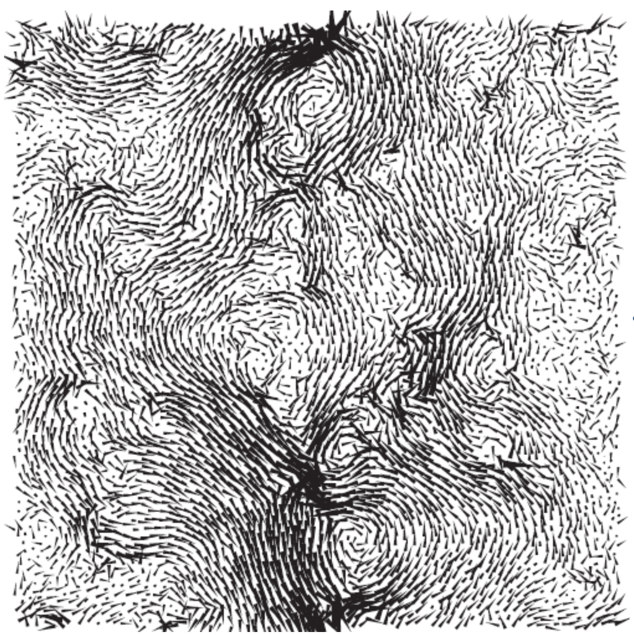

Highly localized modes

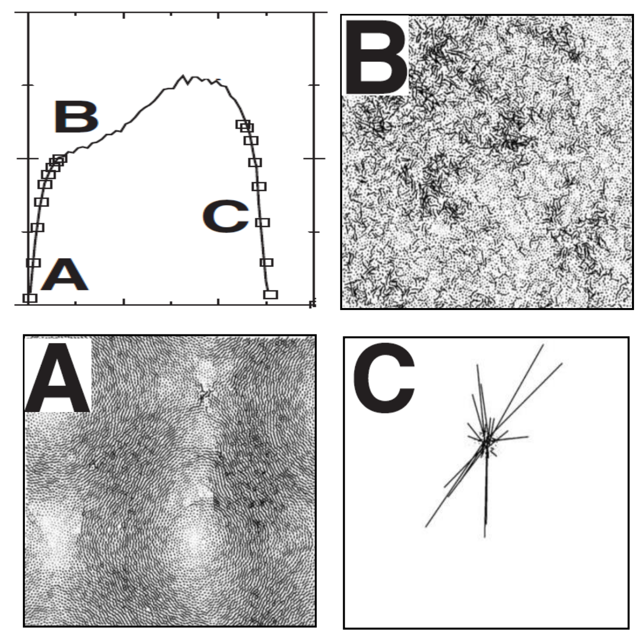
# A question in the present work

- Which vibrational normal modes play a role in energy relaxation process, during non-affine deformation ?

Non-affine relaxation

Vibrational normal modes



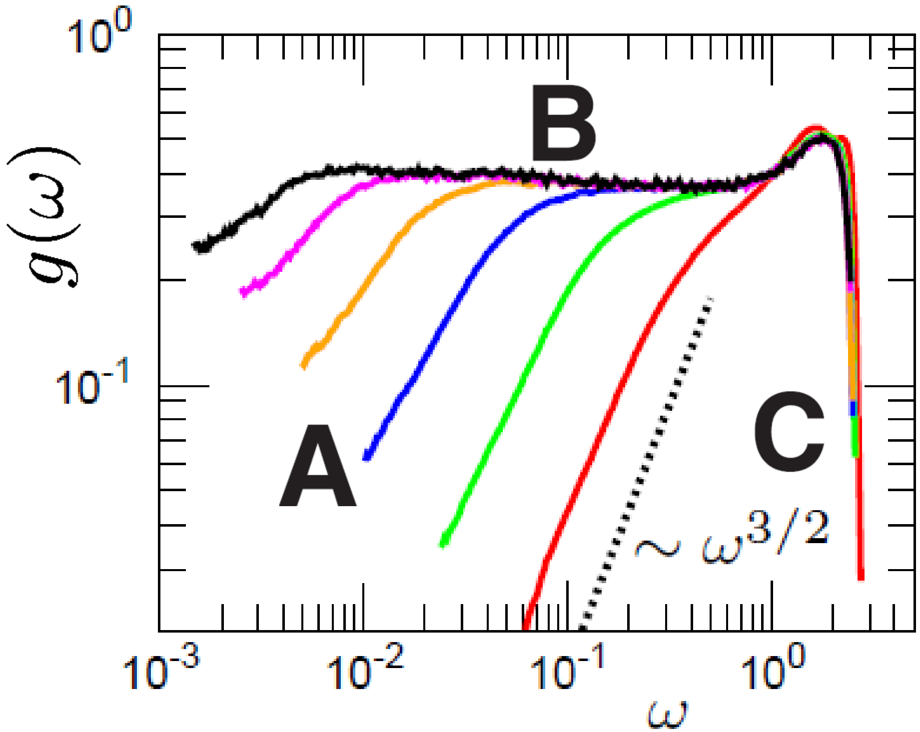


# Present particulate system

- 3 dimensional system
- Harmonic interaction
- Frictionless particles

$$\phi(r_{ij}) = \begin{cases} \frac{\varepsilon}{2}\left(1 - \frac{r_{ij}}{\sigma}\right)^2 & (r_{ij} < \sigma) \\ 0 & (r_{ij} \geq \sigma) \end{cases}$$

- Close to jamming: Packing fraction $\Delta\varphi = \varphi - \varphi_c = 10^{-1}$ to $10^{-6}$




L.E. Silbert et al., PRL(2005), PRE (2009)

**A, Debye-like regime :**

$$\omega < \omega^*$$

**B, Plateau regime :**

$$\omega^* < \omega < \omega^h$$

**C, High frequency regime :**

$$\omega > \omega^h$$

with characteristic frequencies

$$\omega^* \sim \Delta\varphi^{1/2} \quad \omega^h \simeq 1$$

# Vibrational energy of normal mode

- Vibrational energy is separated into two components :
  **(1) compressing/stretching energy** and **(2) sliding energy**
- Sliding motion de-stabilizes the system : $-\delta E^{k\perp} < 0$

M. Wyart et al., PRE (2005)

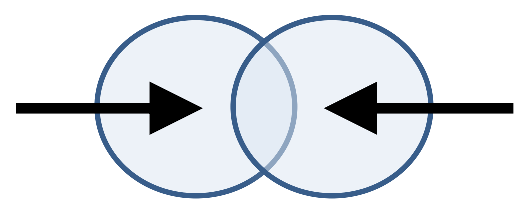
$$\delta E^{k} = \frac{{\omega^{k}}^{2}}{2} = \delta E^{k\parallel} - \delta E^{k\perp}$$

$$= \sum_{(i,j)} \left[ \underbrace{\frac{\phi''(r_{ij})}{2} {\boldsymbol{e}_{ij}^{k\parallel}}^{2}}_{\sim\, {e_{ij}^{k\parallel}}^{2}} + \underbrace{\frac{\phi'(r_{ij})}{2 r_{ij}} {\boldsymbol{e}_{ij}^{k\perp}}^{2}}_{\sim\, -\Delta\varphi \times {e_{ij}^{k\perp}}^{2}} \right]$$

**(1) Compressing/Stretching** **(2) Sliding**

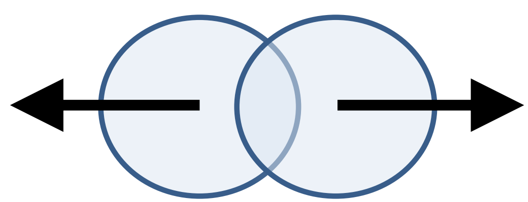
Compressing

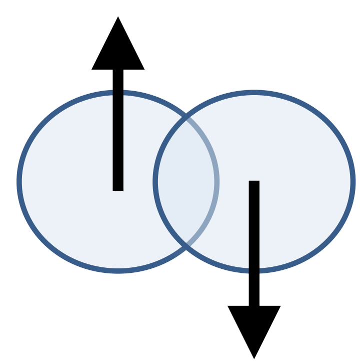
$\boldsymbol{e}_{ij}^{k\parallel} \cdot \boldsymbol{n}_{ij} < 0$



Stretching

$\boldsymbol{e}_{ij}^{k\parallel} \cdot \boldsymbol{n}_{ij} > 0$

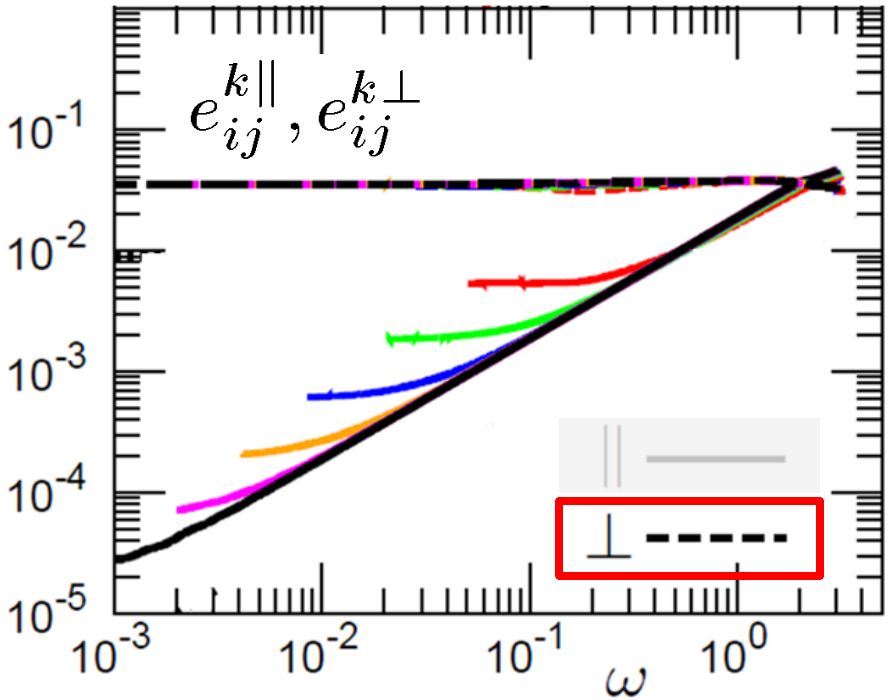


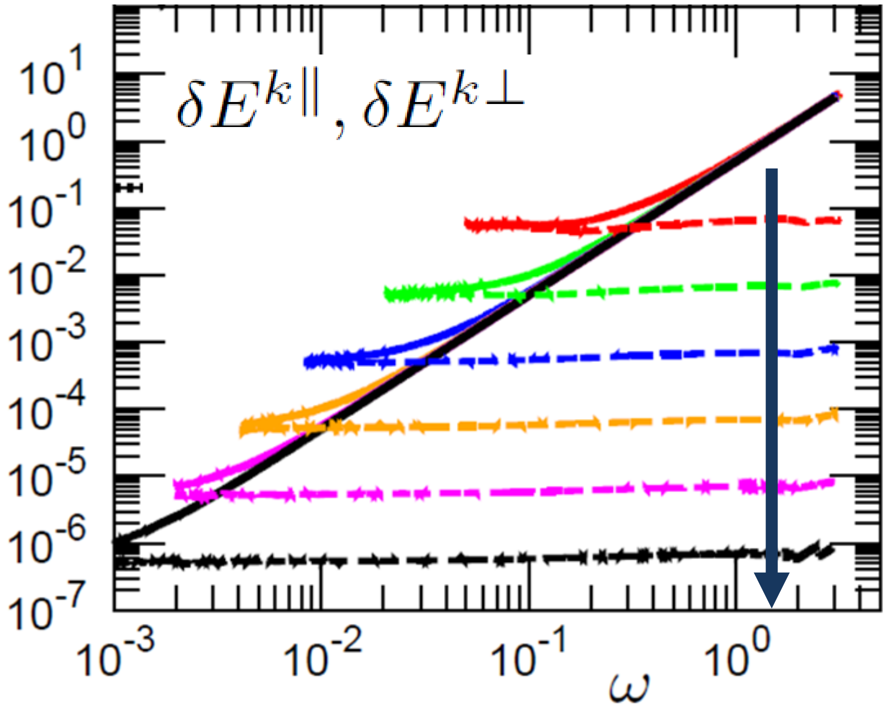


# Sliding motion and energy

- Sliding displacement and energy are **independent of frequency**

$$e_{ij}^{k\perp} \simeq A^{\perp} \text{ (constant)} \qquad \delta E^{k\perp} \sim \Delta\varphi {e_{ij}^{k\perp}}^2 \simeq \Delta\varphi {A^{\perp}}^2$$



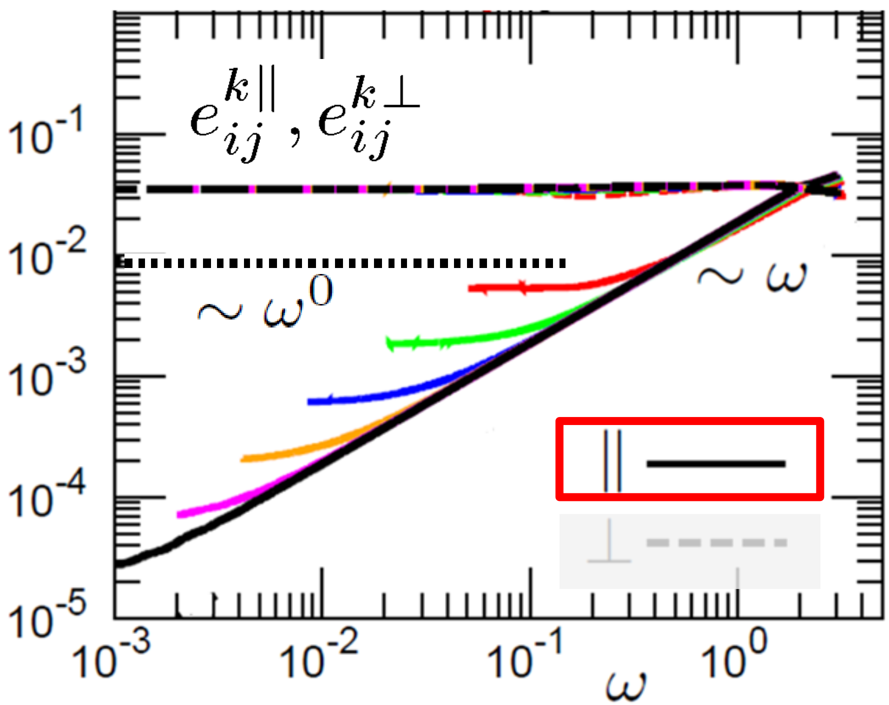
# Compressing/stretching motions and energy

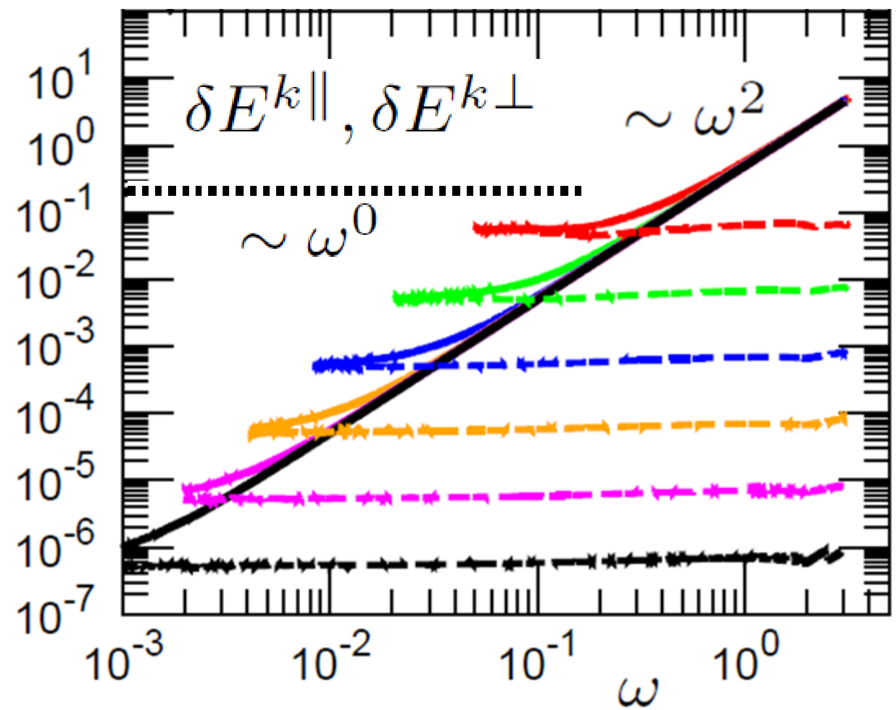
- At high frequencies , $\omega > \omega^*$

$$e_{ij}^{k\|} \sim \delta E^{k\|^{1/2}} \sim \omega \qquad \delta E^{k\|} \simeq \omega^2/2 \gg \delta E^{k\perp}$$

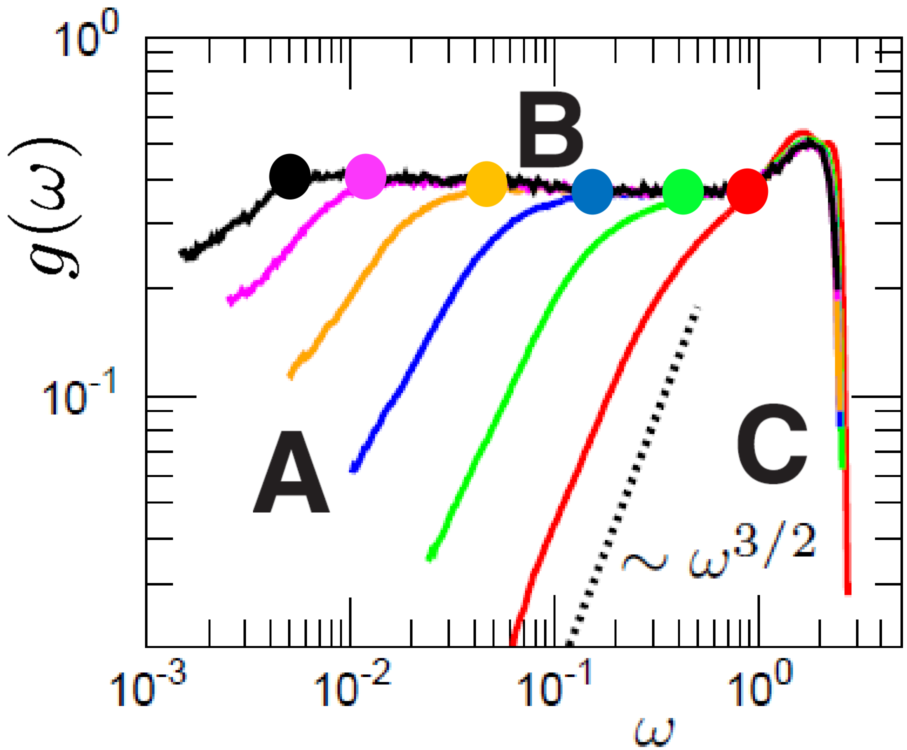
- At low frequencies , $\omega < \omega^*$

$$e_{ij}^{k\|} \sim \Delta\varphi^{1/2}\omega^0 \qquad \delta E^{k\|} \sim \delta E^{k\perp} \sim \Delta\varphi\omega^0$$



# Characterization of frequency $\omega^*$




**B C** : $\omega > \omega^*$

$$\delta E^{k\parallel} \simeq \omega^2/2 \gg \delta E^{k\perp}$$

**A**: $\omega < \omega^*$

$$\delta E^{k\parallel} \sim \delta E^{k\perp} \sim \omega^0$$

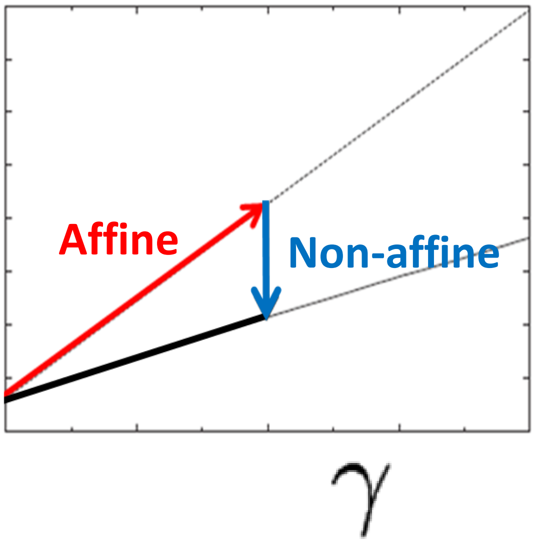
- $\omega^*$ is a point where **the sliding energy starts to play a role !**

At $\omega = \omega^*$, $\delta E^{k\parallel} \simeq \frac{\omega^{*2}}{2} \sim \delta E^{k\perp} \sim \Delta\varphi$

$$\Rightarrow \omega^* \sim \delta E^{k\perp 1/2} \sim \Delta\varphi^{1/2}$$

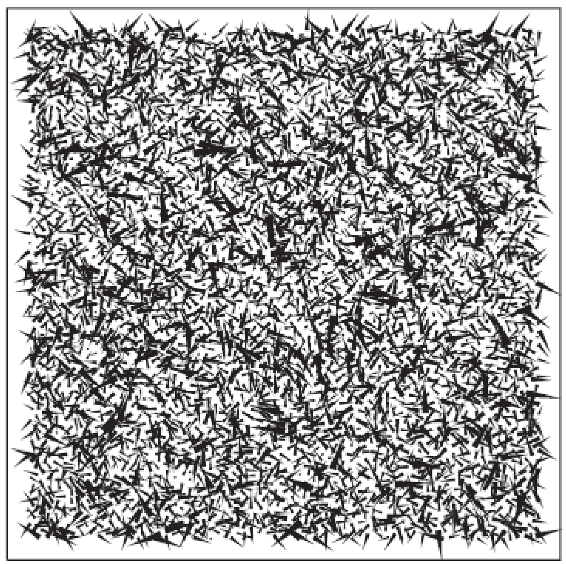
# Normal-mode decomposition of non-affine modulus

Stress-Strain curve




**Force field** is induced by affine deformation

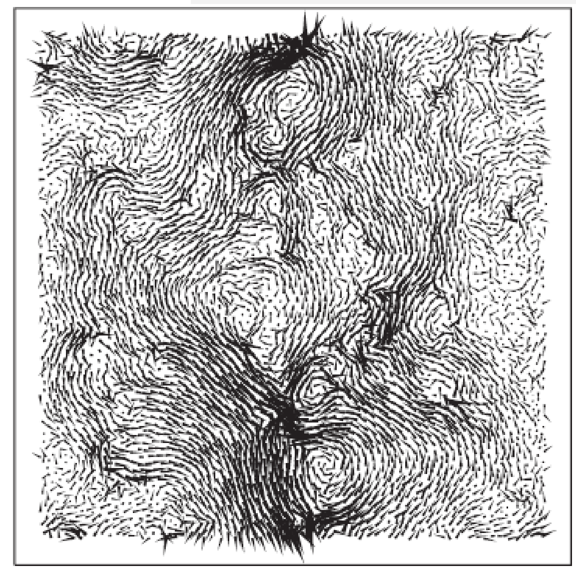
$$\boldsymbol{\Sigma} = \frac{\partial \boldsymbol{F}}{\partial \gamma}$$



**Non-affine displacements** are driven by the force field

$$\delta \boldsymbol{R}_{\mathrm{na}} = H^{-1} \cdot \boldsymbol{\Sigma}$$

Linear response to the force field



C.E. Maloney, PRL (2006)

**Non-affine modulus**

$$M_N = \frac{1}{V} \boldsymbol{\Sigma} \cdot \delta \boldsymbol{R}_{\mathrm{na}}$$

**Energy relaxation** (force times displacement) during the non-affine deformation

# Normal-mode decomposition of non-affine modulus

- Decompose non-affine modulus into each mode k contribution
- We can understand which modes play an important role in energy relaxation during non-affine deformation

**Force field** induced by affine deformation

$$\boldsymbol{\Sigma} = \sum_{k=1}^{3N-3} \Sigma^k \boldsymbol{e}^k$$

**Non-affine displacement** driven by force field

$$\delta \boldsymbol{R}_{\mathrm{na}} = \sum_{k=1}^{3N-3} \delta R_{\mathrm{na}}^k \boldsymbol{e}^k = \sum_{k=1}^{3N-3} \frac{\Sigma^k}{{\omega^k}^2} \boldsymbol{e}^k$$

**Non-affine modulus**: Energy relaxation during non-affine deformation

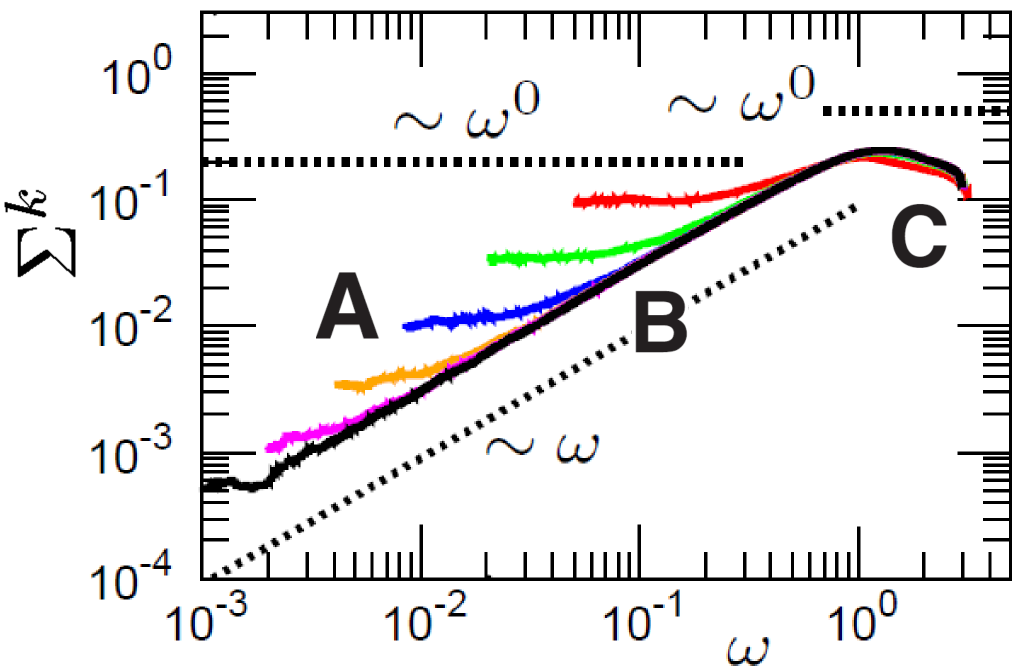
$$M_N = \frac{1}{V} \sum_{k=1}^{3N-3} M_N^k = \frac{1}{V} \sum_{k=1}^{3N-3} \Sigma^k \delta R_{\mathrm{na}}^k$$

Lemaitre and Maloney, J. Stat. Phys. (2006)

# Force field induced by affine deformation

Under (affine) shear deformation

- Force field is induced mainly along normal modes in the high freqeuncy regime C : $\omega > \omega^h$
- Forces are related to compressing/stretching vibrational amplitude
- Crossover between A and B at $\omega^*$ is caused by the sliding energy



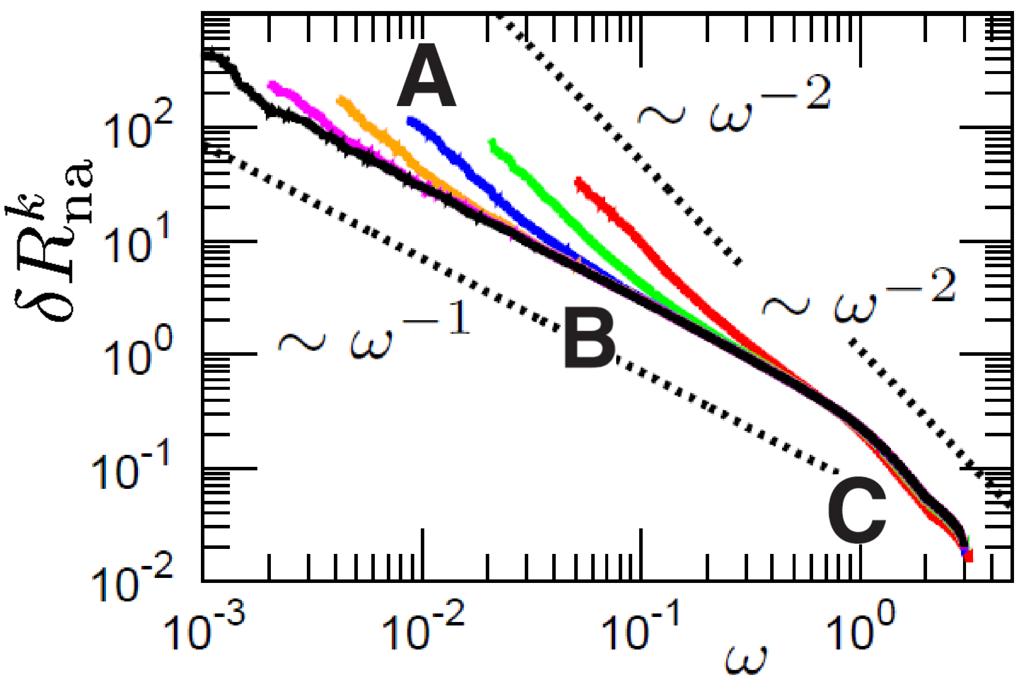

$$\Sigma^k \left( \approx \phi''(r_{ij}) e_{ij}^{k\|} \right)$$

$$\sim \begin{cases} \omega^0 & (\omega > \omega^h) \text{ C} \\ \omega & (\omega^* < \omega < \omega^h) \text{ B} \\ \omega^0 & (\omega < \omega^*) \text{ A} \end{cases}$$

# Displacement field driven by force field

Under (affine) shear deformation

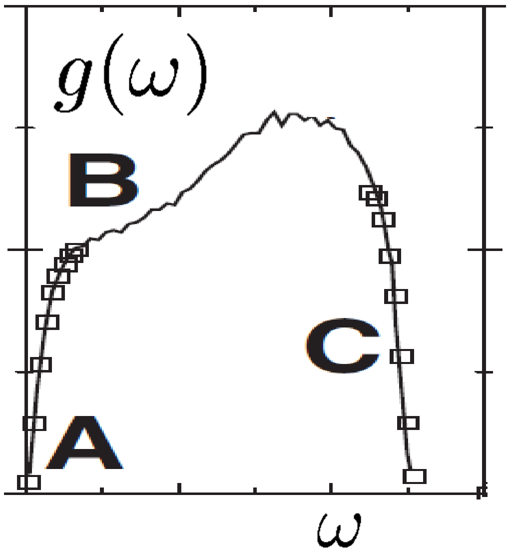
- Non-affine displacement field (driven by force field) occurs mainly along normal modes in the Debye-like regime A : $\omega < \omega^*$
- At $\omega < \omega^*$, the sliding energy drives the displacement field
- High frequency, energetic modes at $\omega > \omega^h$ are little excited

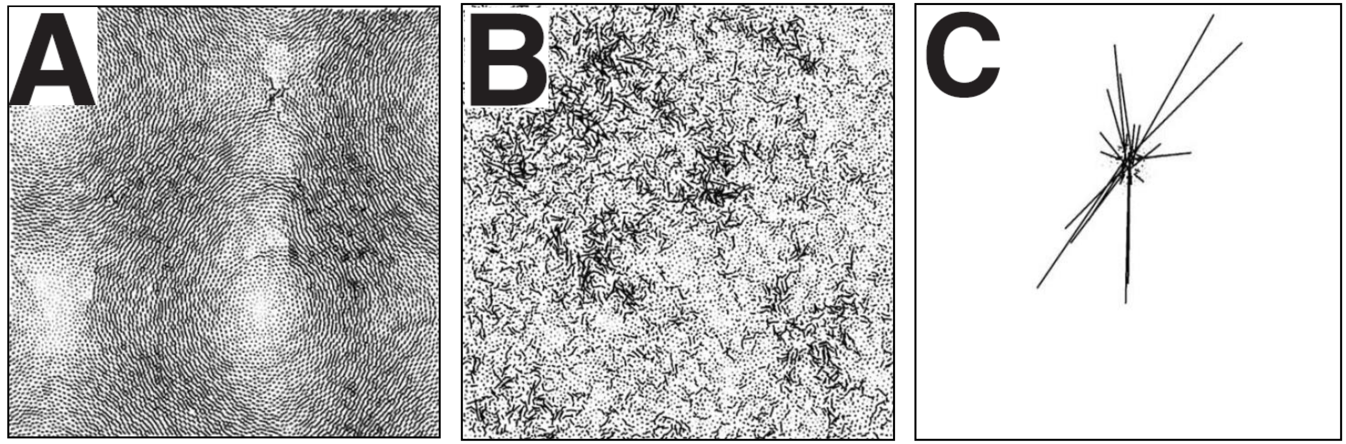



$$\delta R^k_{\mathrm{na}} = \frac{\Sigma^k}{{\omega^k}^2}$$

$$\sim \begin{cases} \omega^{-2} & (\omega > \omega^h)\ \mathbf{C} \\ \omega^{-1} & (\omega^* < \omega < \omega^h)\ \mathbf{B} \\ \omega^{-2} & (\omega < \omega^*)\ \mathbf{A} \end{cases}$$

# Force and displacement fields



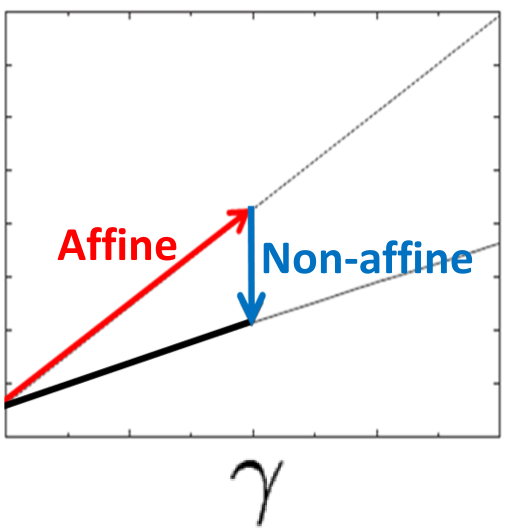



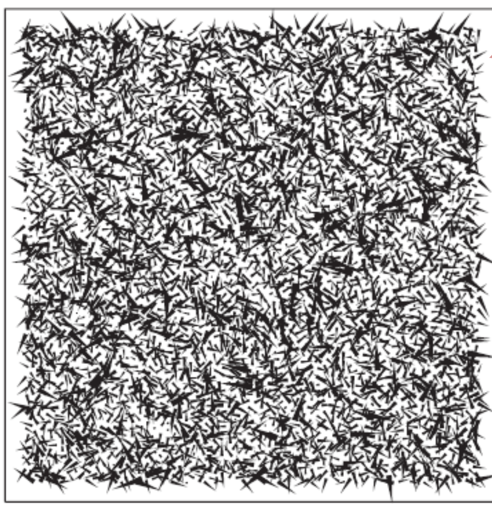

Plane-wave-like modes

Filamentary extended modes

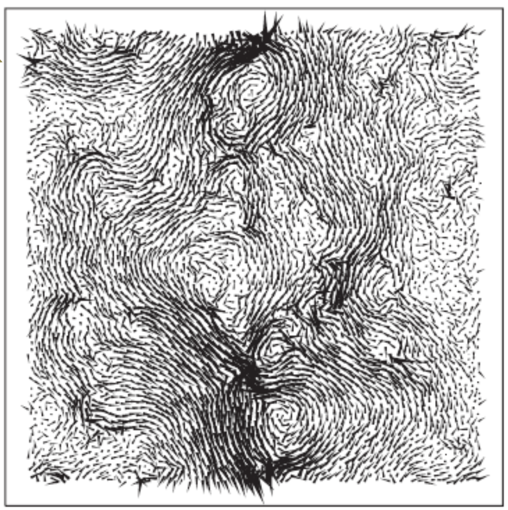
Highly localized modes

Stress-strain curve



**Force field:** Random distribution with short-range correlation

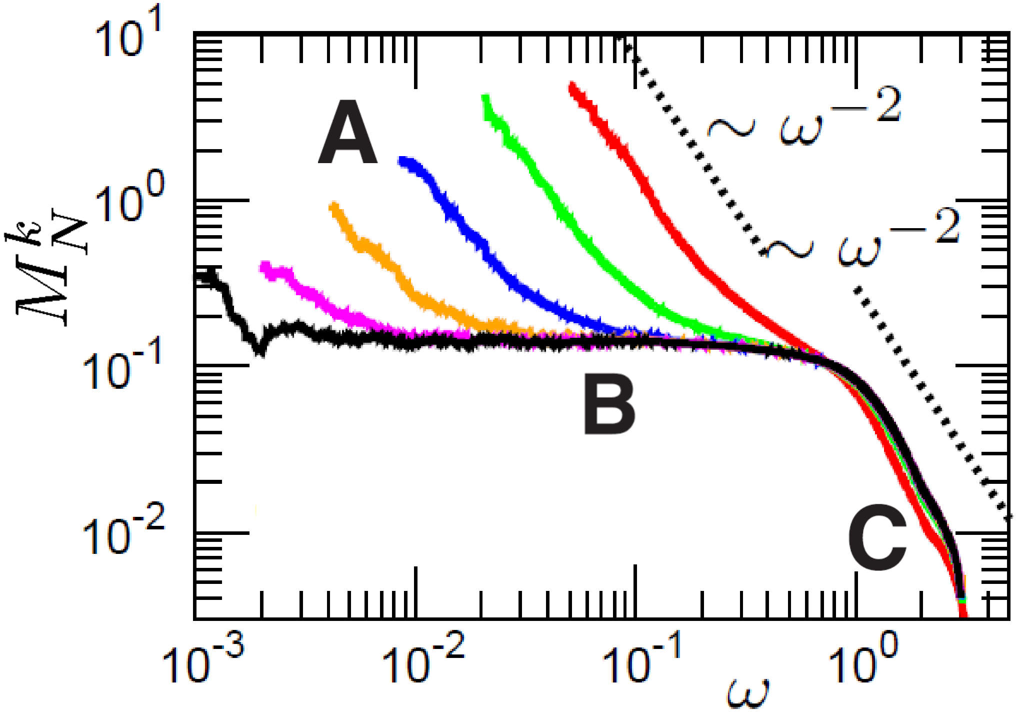


**Displacement field:** Vortex-like structure with long-range correlation

# Non-affine modulus – Energy relaxation

**Non-affine modulus**: Energy relaxation during non-affine deformation

$$M_N^k = \Sigma^k \times \delta R_{\mathrm{na}}^k \sim \begin{cases} \omega^{-2} & (\omega > \omega^h) \ \textbf{C} \\ \omega^{0} & (\omega^* < \omega < \omega^h) \ \textbf{B} \\ \omega^{-2} & (\omega < \omega^*) \ \textbf{A} \end{cases}$$



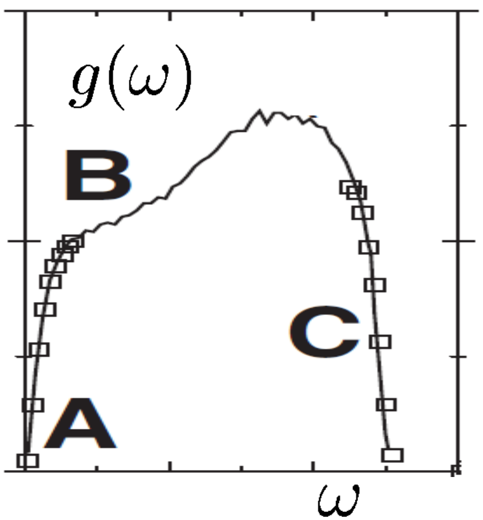

**A, Debye-like regime :**
Energy relaxation is enhanced, due to the sliding motions

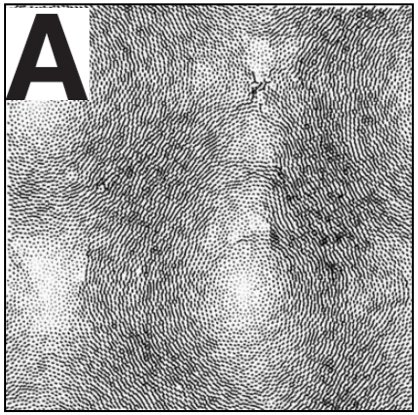
**B, Plateau regime :**
Mode contributions are independent of frequency

**C, High frequency regime :**
Few contributions

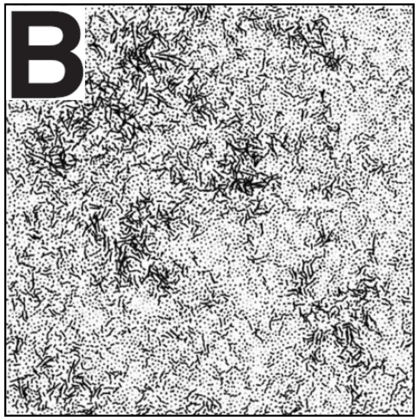
# Our main conclusion

- Affine deformation induces the **force field** mainly along normal modes in the **high frequency regime C**.
- The force field drives the **non-affine displacement field** mainly along modes in the low frequency, **Debye-like regime A**.
- **Energy relaxations (non-affine modulus)** occur mainly in **Debye-like regime A and plateau regime B**, whereas those do not in regime C.
- In **Debye regime A**, the **sliding energy** destabilizes the system, inducing further energy relaxations.

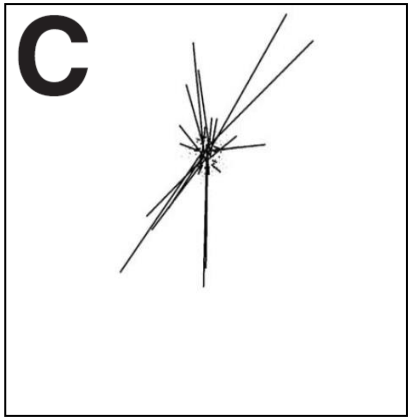



Plane-wave-like modes




Filamentary extended modes




Highly localized modes

# Thank you for your attention

In collaboration with

Kuni Saitoh

Leo Silbert

- “Elastic Moduli and Vibrational Modes in Jammed Particulate Packings”, H. Mizuno, K. Saitoh, and L. E. Silbert, submitted to *Physical Review E.*